New Opportunities in Surface and Interfacial Science

Summary of the Workshop on "In-Situ Characterization of Surface and Interface Structures and Processes“, and APS Upgrade Planning Meeting

Paul Zschack

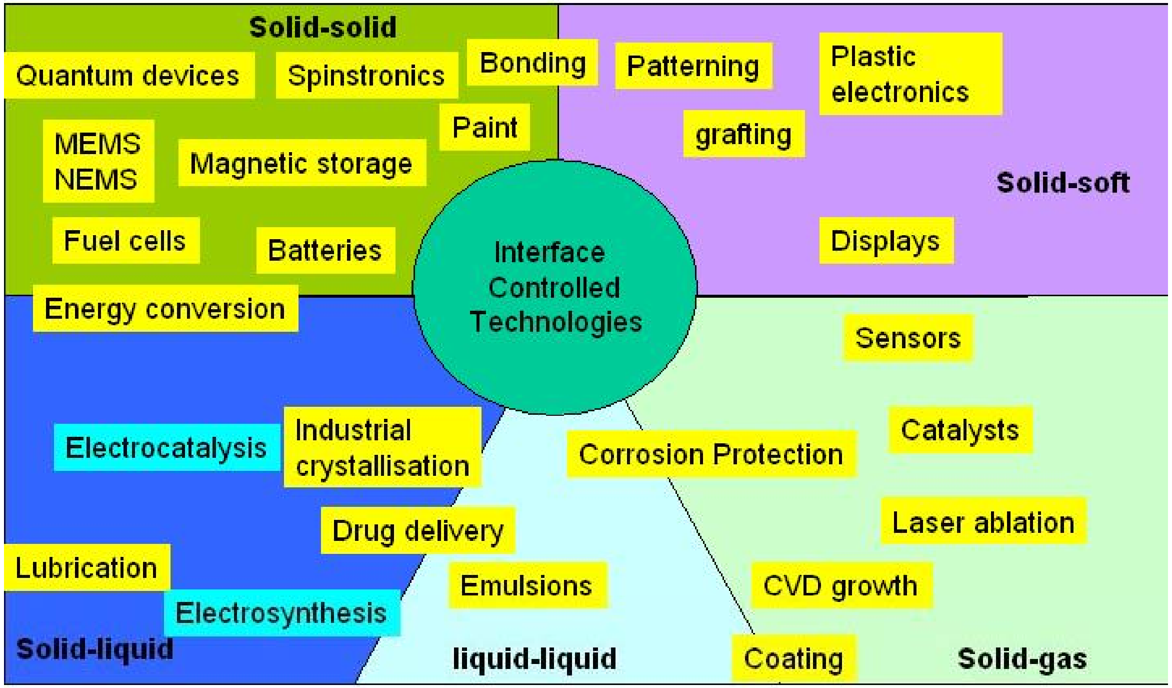
APS X-Ray Science Division

A U.S. Department of Energy laboratory managed by The University of Chicago

Surface & Interface Science Today

- Energy
- Communications
- Medicine
- Catalysis
- Geo-chemistry
- Environmental Science
- Nano-science

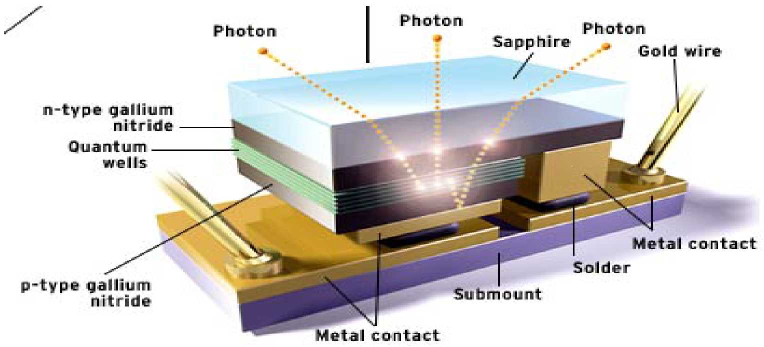
- Magnetic Materials
- Thermoelectrics
- Photonics
- Spintronics
- Ferroelectrics
- Fuel Cells
- Semiconductors



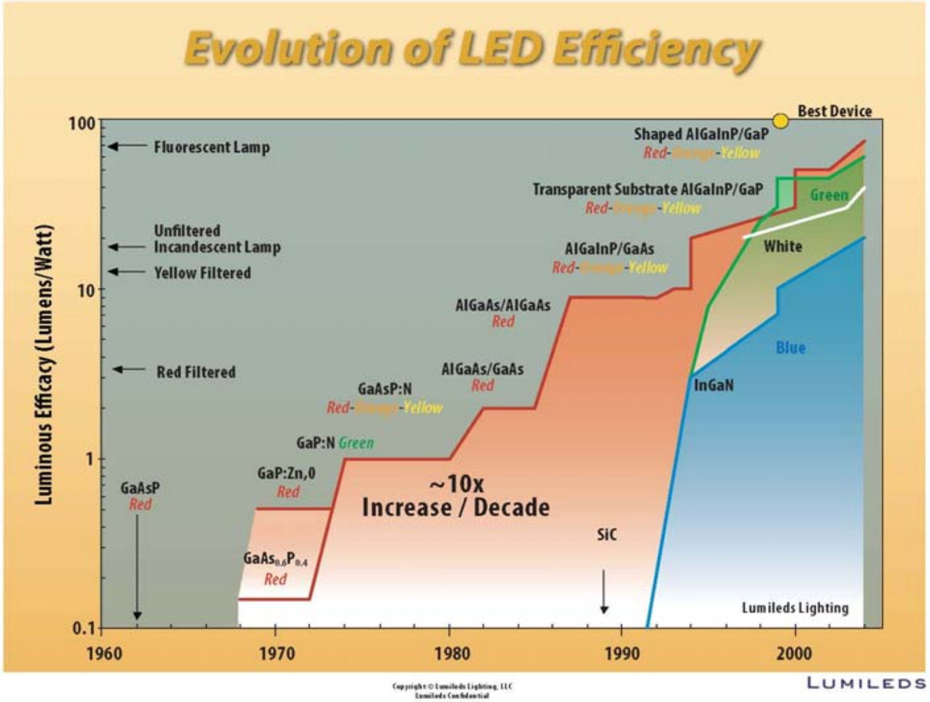
J.F. van der Veen, PSI Institute, Switz. (2005)

For APS: Clearly identified potential impact in many of these areas

Impact in Energy



- Lighting accounts for ~20% of global electricity consumption.
- If 150 lm/W white source developed
  - ~ 50% power conversion (or “wall-plug”) efficiency
  - e.g., today’s best red/infrared III-V LED and laser diode performance
- Potential 10% reduction in global electricity consumption
  - ~1000 TWh/year in energy (or $100B/year in cost)
  - 200M tons/year global carbon emissions

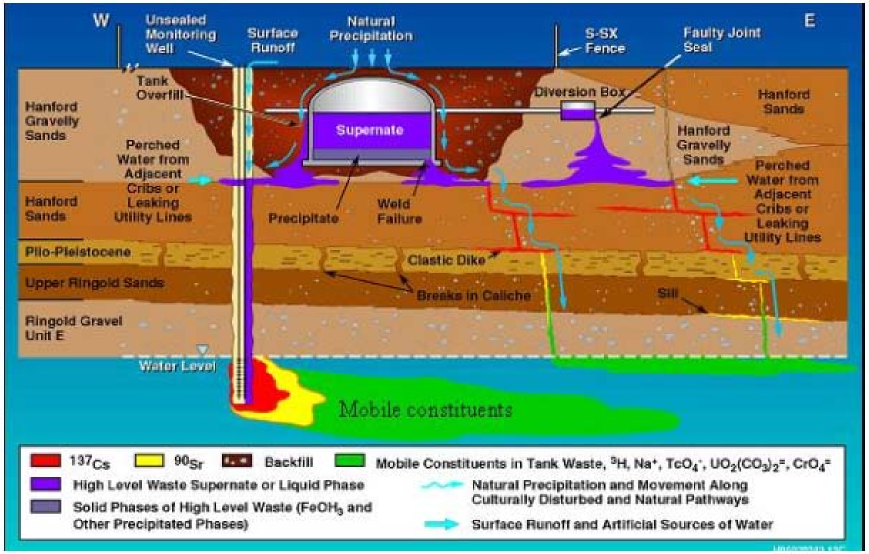


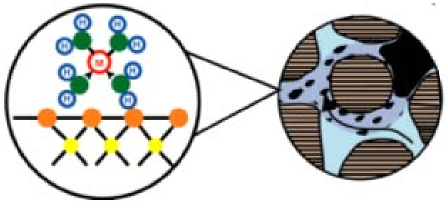
Anneli Munkholm, LUMILEDS Lighting LLC (2005)

Impact in Environmental Science

Contamination and Migration at the Hanford Site

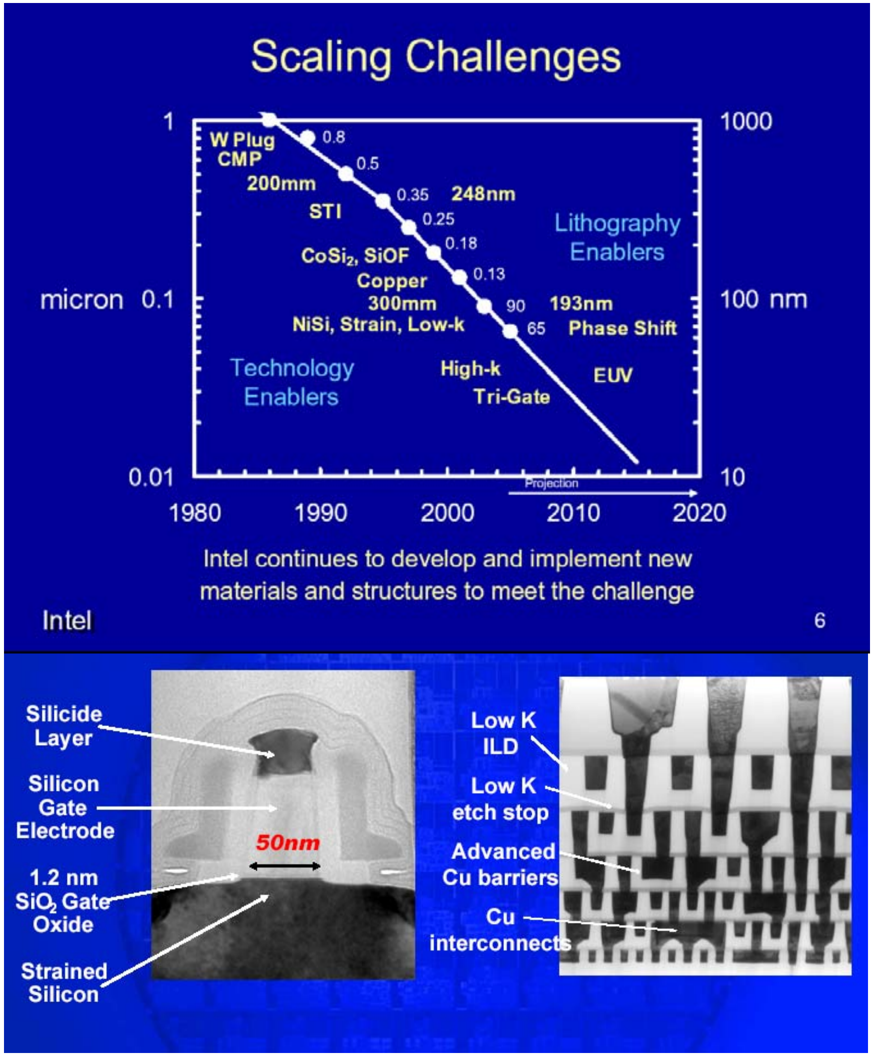
From: *Molecular Environmental Science: An Assessment of Research Accomplishments, Available Synchrotron Radiation Facilities, and Needs*, by G. E. Brown, Jr. et al., 2003



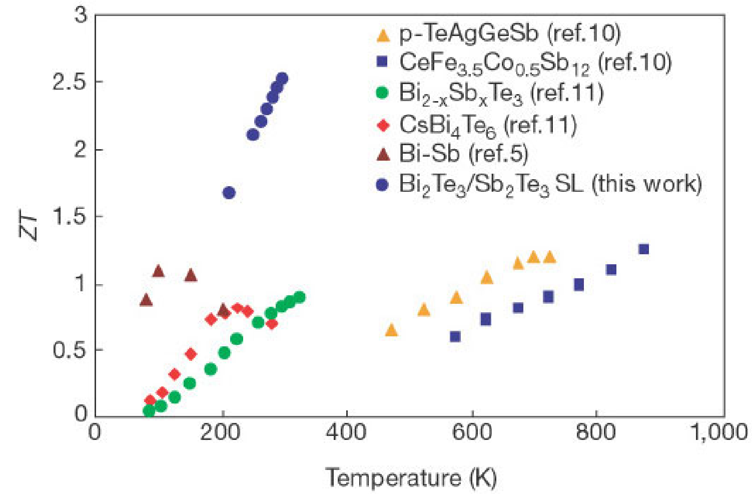


Transport is controlled by specific interactions of ions with mineral-water interfaces (micas, clays, silicates, oxides, carbonates…)

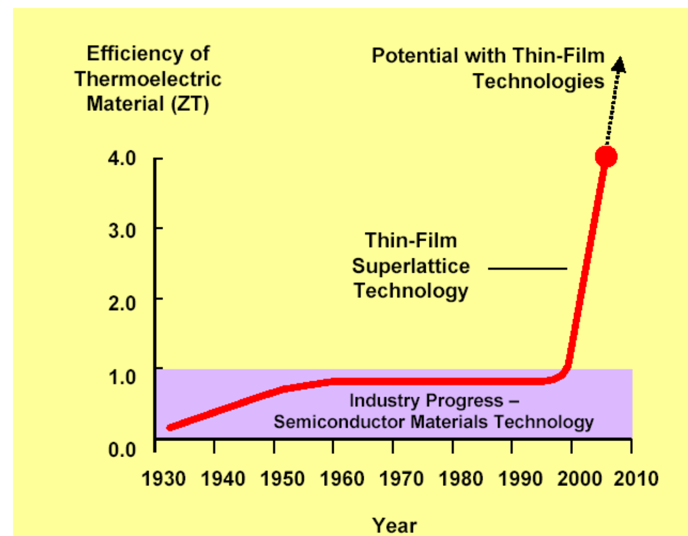
Impact today and tomorrow



Mark Bohr, Intel corp. (2004)



R. Venkatasubramanian, et.al. Nature **413**, 597-602 (2001)



J. Fairbanks, Office of FreedomCAR, US DOE (2004)

Workshop at APS

Workshop on In-Situ Characterization of Surface & Interface Structures and Processes

September 8-9, 2005 Advanced Photon Source Argonne National Laboratory, Argonne, Illinois 60439

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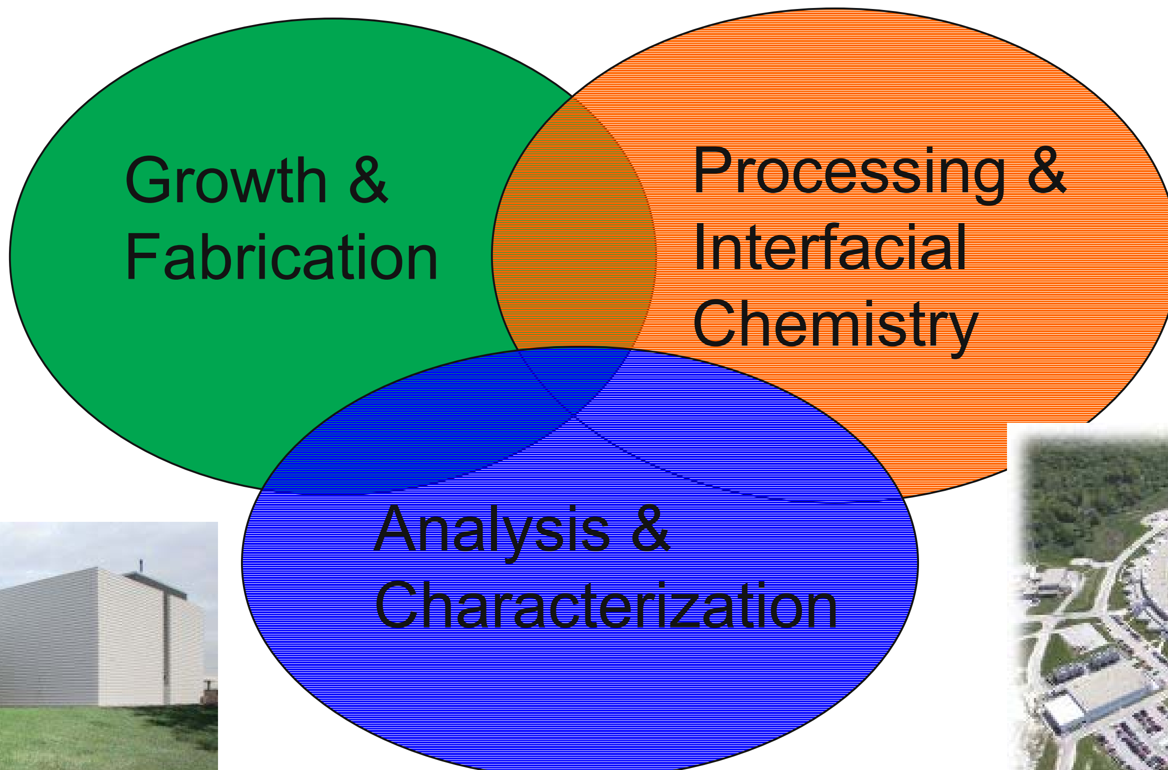
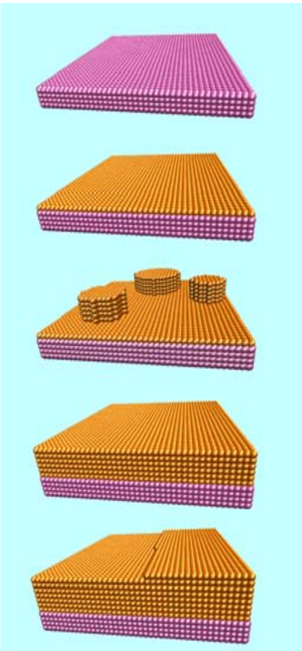
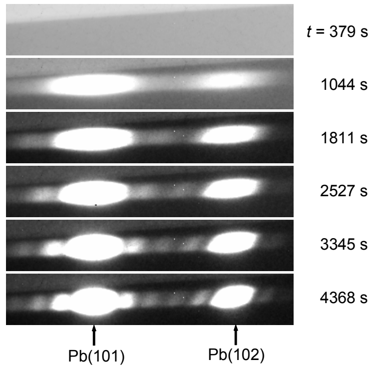
http://surface-interface.aps.anl.gov

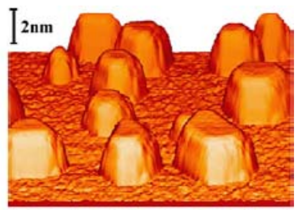


Workshop on In-Situ Characterization of Surface & Interface Structures and Processes

Real-time x-ray growth at 180 K



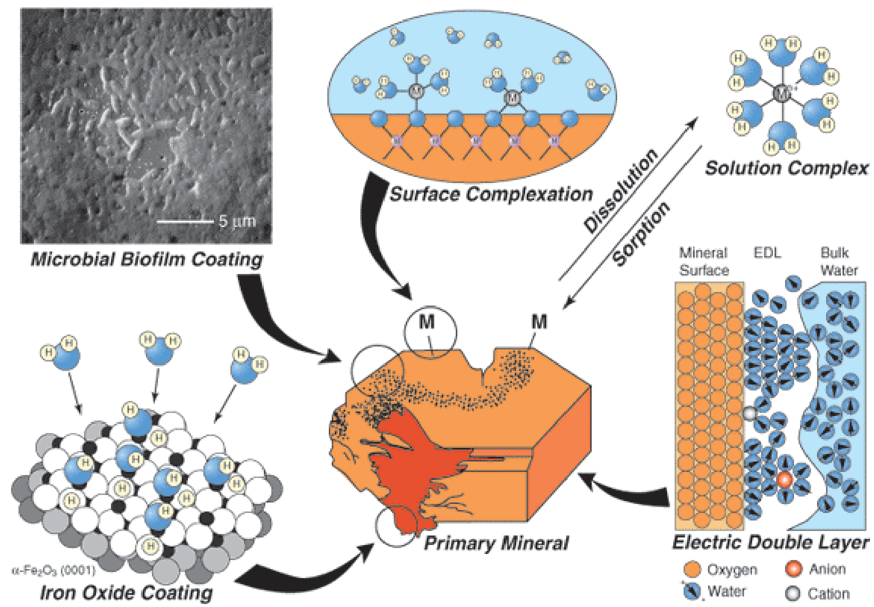




Magic islands: Tringides, et al. Surf. Sci. 493, 526 (2001)

T.C. Chiang, Univ of Illinois (2005)

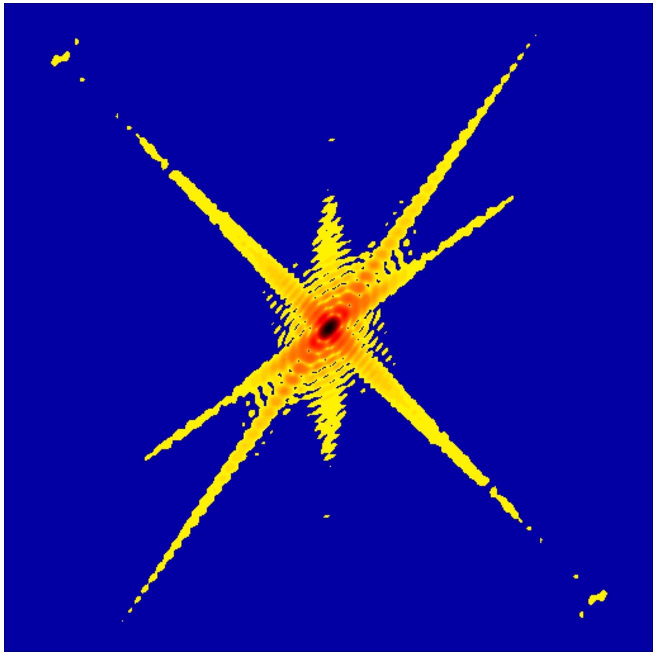
- ***Interfacial Chemistry*** – including geochemical and environmental processes, electrochemistry, fuel cells, and catalysis



G.E. Brown, Jr. (2001) How minerals react with water, *Science* 294, 67-69.

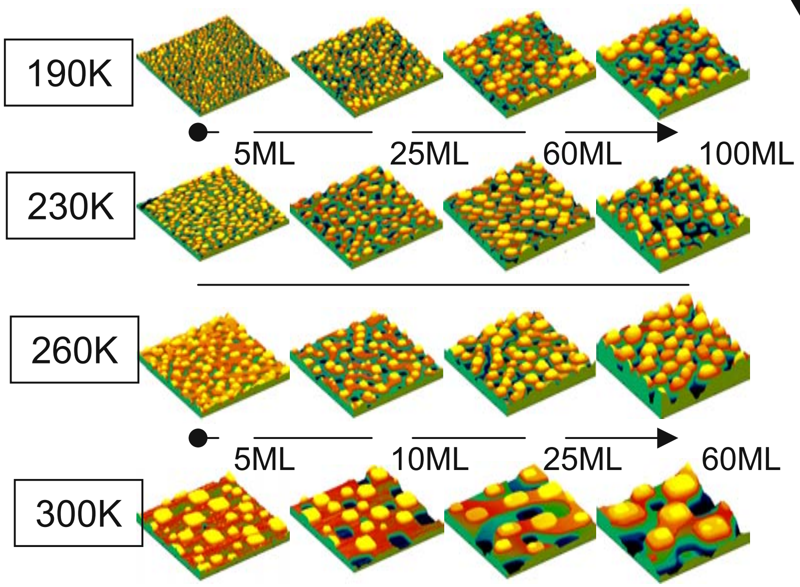
- ***Integrated Materials Fabrication*** – including nanoscale assembly, growth, and oxidation

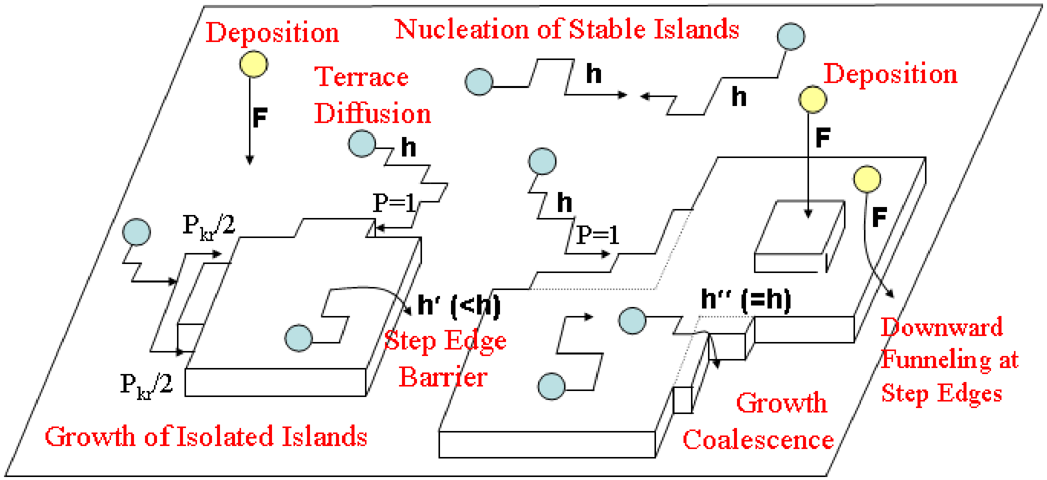
Workshop on In-Situ Characterization of Surface & Interface Structures and Processes



I.K. Robinson, Univ of Illinois (2004)

- ***Analysis & Characterization*** – including phase correction algorithms, coherent diffraction, imaging and modeling.





Jim Evans, Iowa State Univ (2005)

Workshop Recommendations

Provide state of the art beamline facilities and infrastructure to support current forefront research efforts, and expand facilities to enable anticipated new opportunities.

Increase the number of XOR staff scientists whose research encompasses the area of surface and interface scattering.

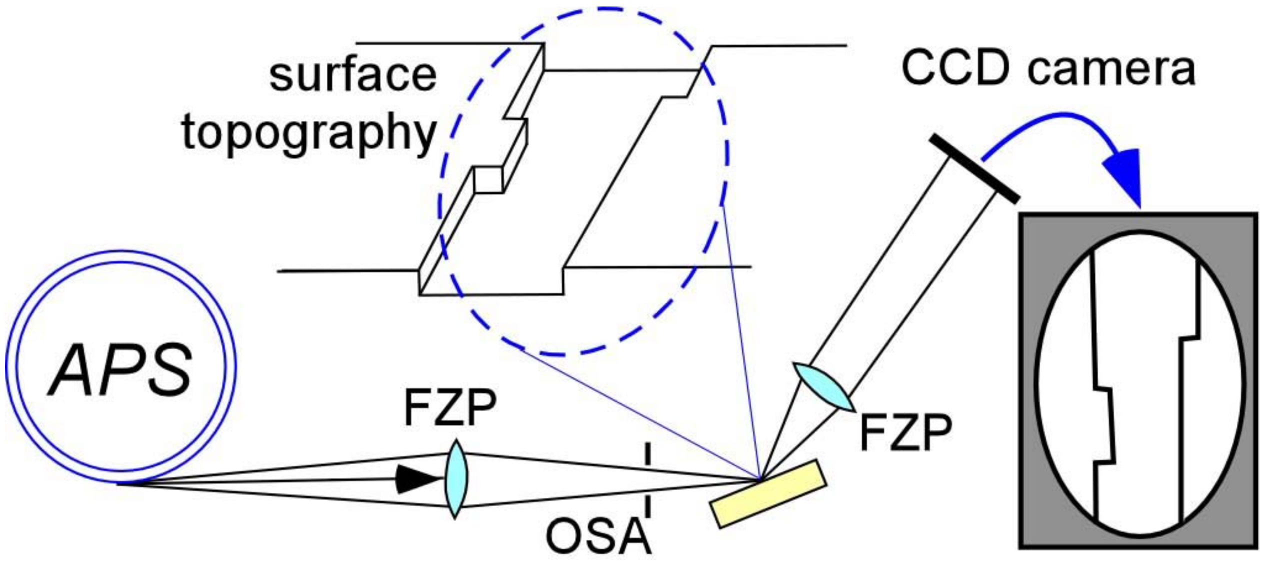
Establish a formal mechanism to get the advice and recommendations of the research community in the development of these research facilities.

Encourage and support user community efforts to develop a proposal for a greenfield facility for materials creation, processing, and in-situ surface and interface and characterization.

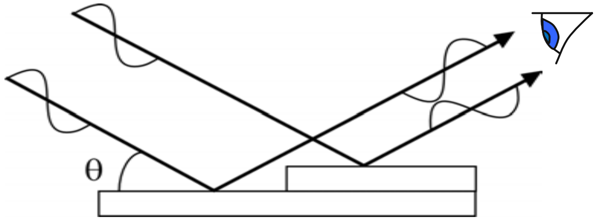
Develop suitable access modes and policies to encourage strong *in-situ* characterization and processing programs.

Enable access to other capabilities at ANL.

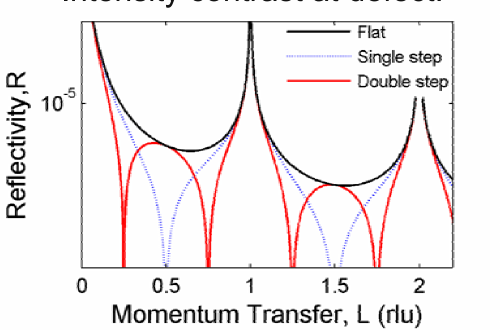
X-ray Reflection Interface Microscopy (XRIM)



Phase contrast mechanism:



Intensity contrast at defect:



Characteristics:

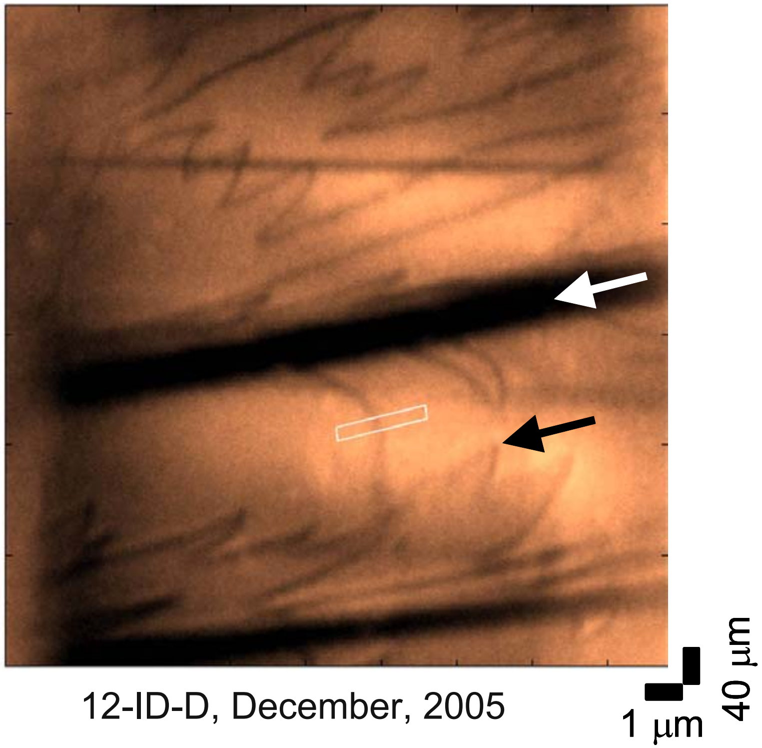
→ Strong contrast at defects (~100%), but weak reflected beam intensity ($R < 10^{-5}$)

→ Sub-nm vertical sensitivity, but modest lateral resolution (200 nm to date),

*P. Fenter, C. Park, Z. Zhang, and S. Wang, in review (2006)

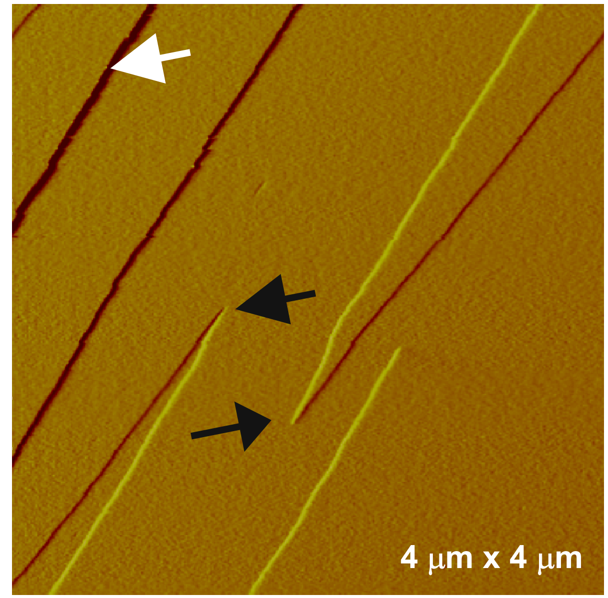
Observation of Step Distributions with XRIM

Step distributions on orthoclase (001)



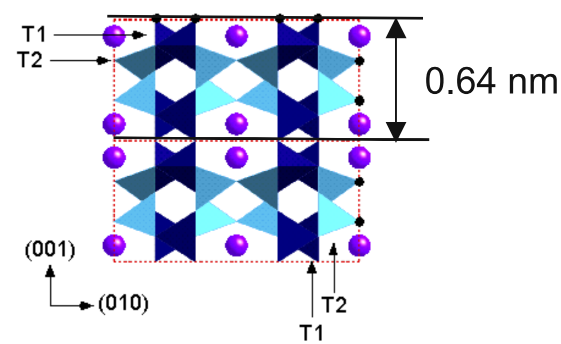
12-ID-D, December, 2005

AFM of orthoclase, $KAlSi_3O_8$ (001)



Teng et al., GCA **65,** 3459-3474 (2001)

Elementary step structure:



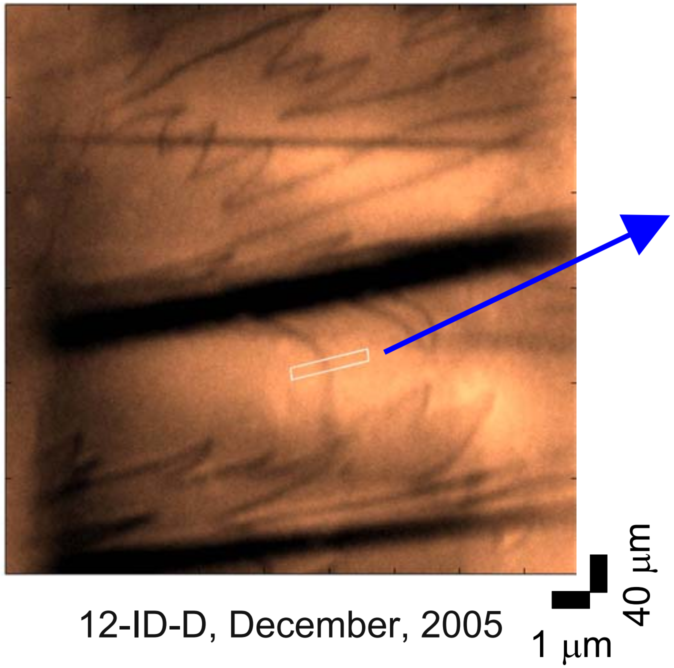
Imaging Conditions:

- $\theta = 1.4°$
- E = 10 keV
- L = 0.25 rlu (Q = 0.24 Å^{-1})
- Sample held in air

*P. Fenter, C. Park, Z. Zhang, and S. Wang, in review (2006)

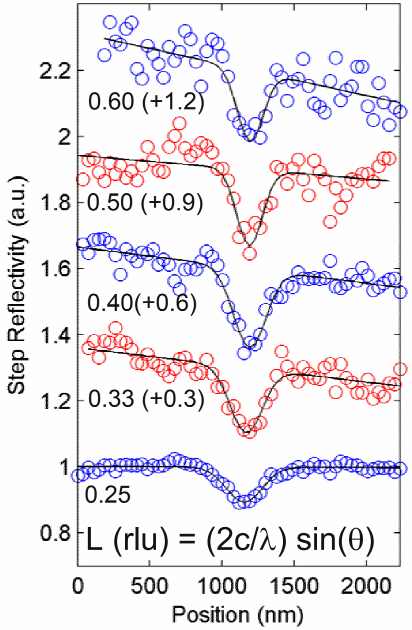
Step Identification with Phase Contrast

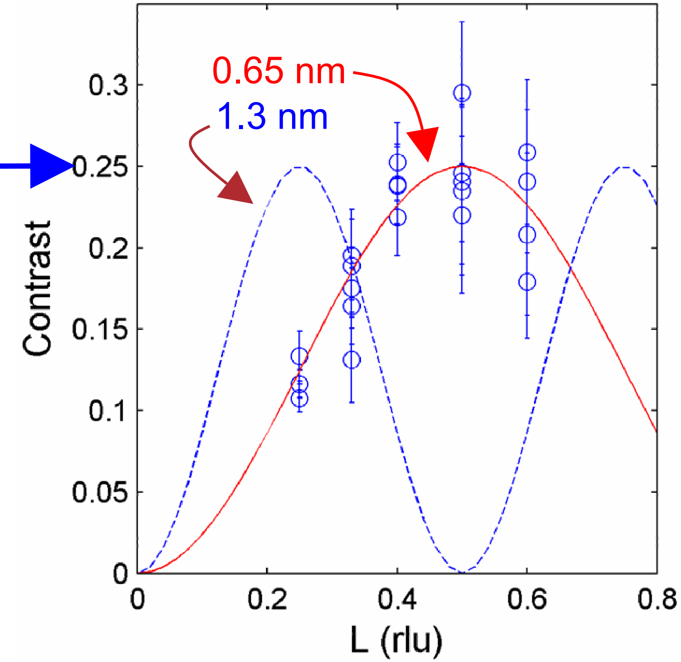
Step distributions on orthoclase (001)



12-ID-D, December, 2005

Identification of step height:





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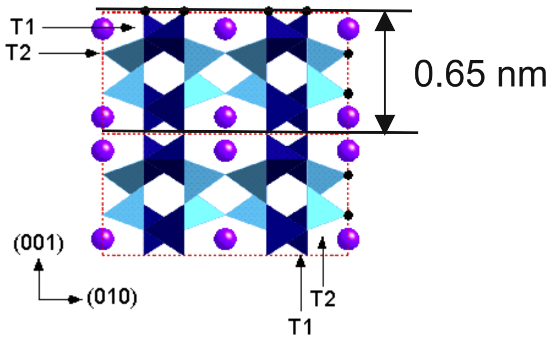


Sub-nm vertical sensitivity:

- derived through variation of phase contrast
- highlighted feature is identified as a monomolecular step

*P. Fenter, C. Park, Z. Zhang, and S. Wang, in review (2006)

New Opportunities with XRIM

A new capability combining:

- exquisite structural sensitivity derived from interfacial X-ray scattering
- high spatial resolution derived from X-ray microscopy

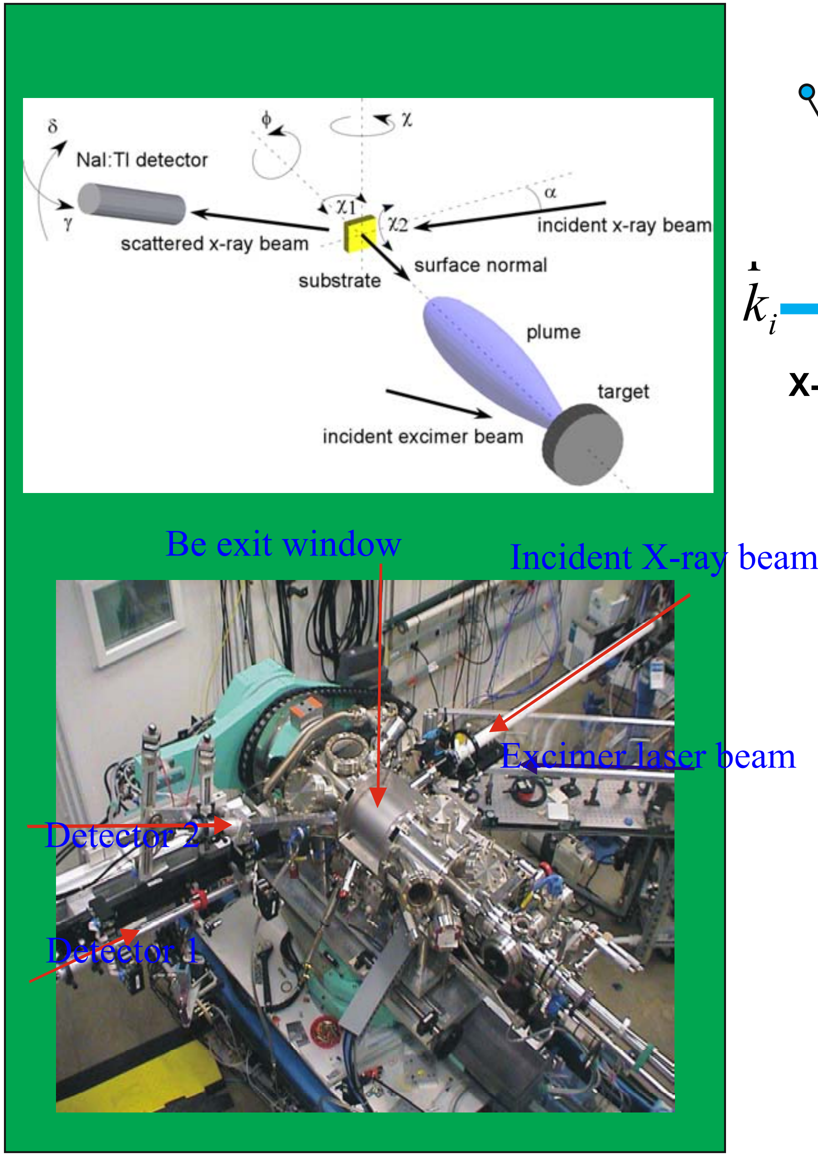
A *non-invasive* structural tool (no probe tip):

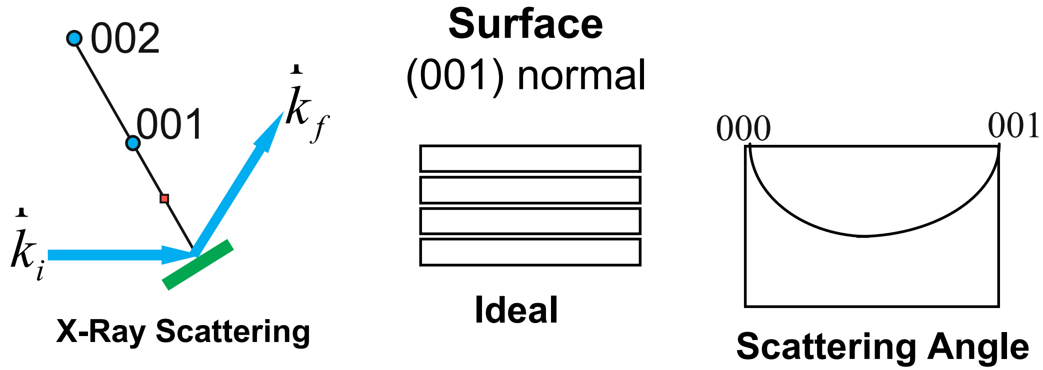
- reactions in aggressive chemical conditions (extreme pH, corrosive gases)
- elevated temperature
- buried interfaces

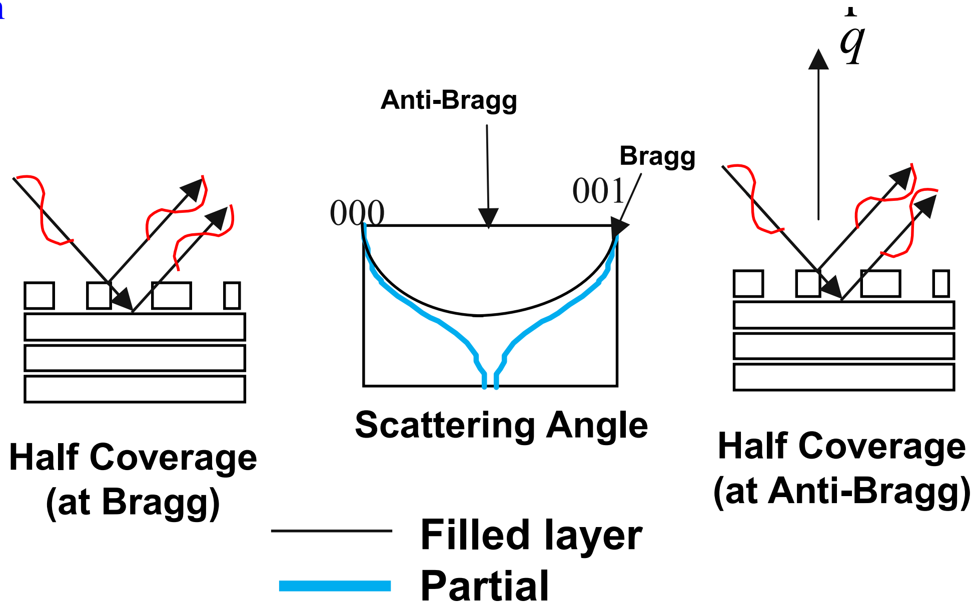
In-situ, real-time observations of interfacial reactions:

- geochemical reactions at solid-liquid interfaces
  - dissolution
  - heterogeneous growth
  - nucleation site distribution (terrace vs. step)
  - phase determination (e.g., calcite vs. aragonite for $CaCO_3$)
  - nano-particle hetero-epitaxy
- materials growth (MOCVD, MBE, oxides)
- corrosion and oxidation
- ferroelectric domain switching
- magnetic domain structures

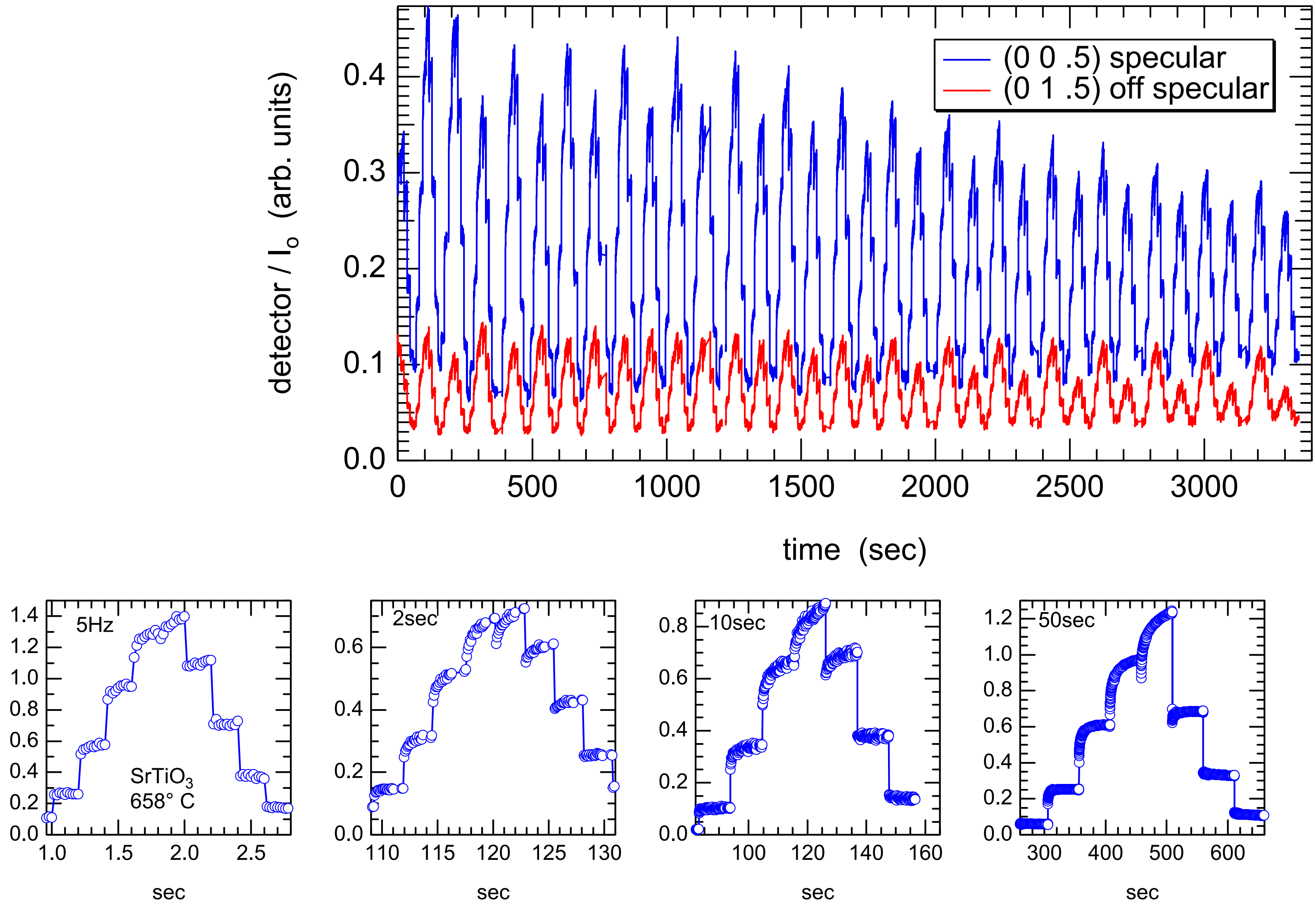
Time-resolved Growth – Pulsed Laser Deposition (PLD)







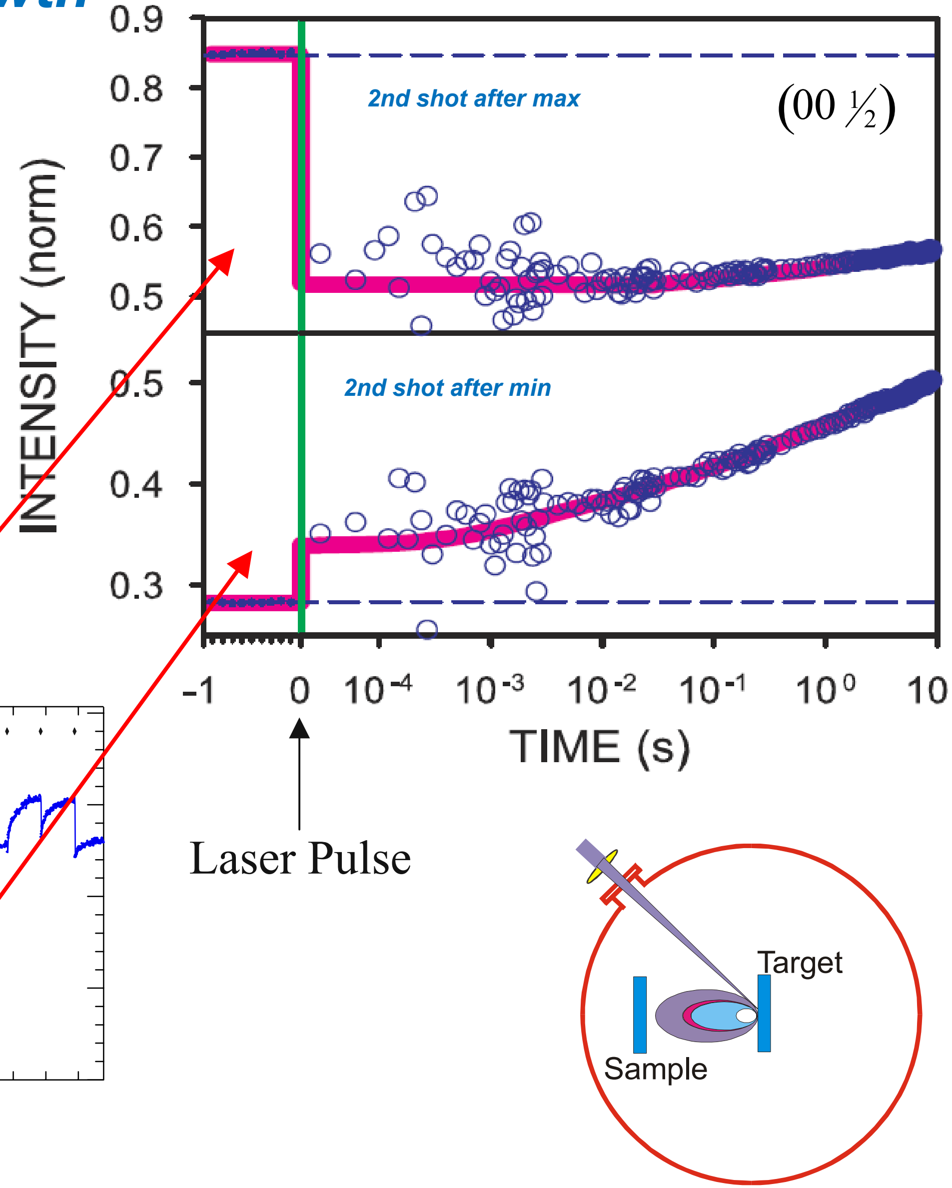
Self-similarity in Time Domain - Homoepitaxy STO

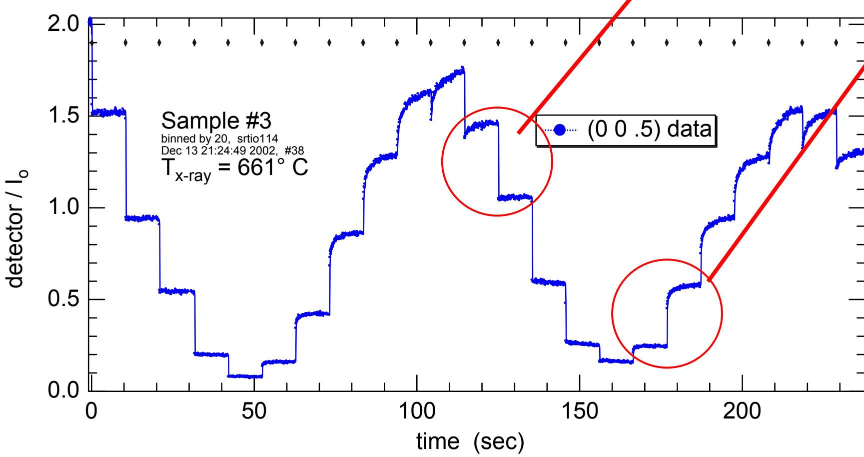


Dwell times vary by x 250 but growth curves appear self-similar

Fast, non-equilibrium growth

- <u>Most</u> of the material moves down a layer in first few μs
- The obvious thermal annealing only affects < 20% of the material deposited.
- Traditional annealing models miss most of the physics.
- Transverse length scale depends upon Temperature and the dwell time between laser shots.





Tischler, et.al. *Phys Rev Lett* **96** (22) 226104 (2006)

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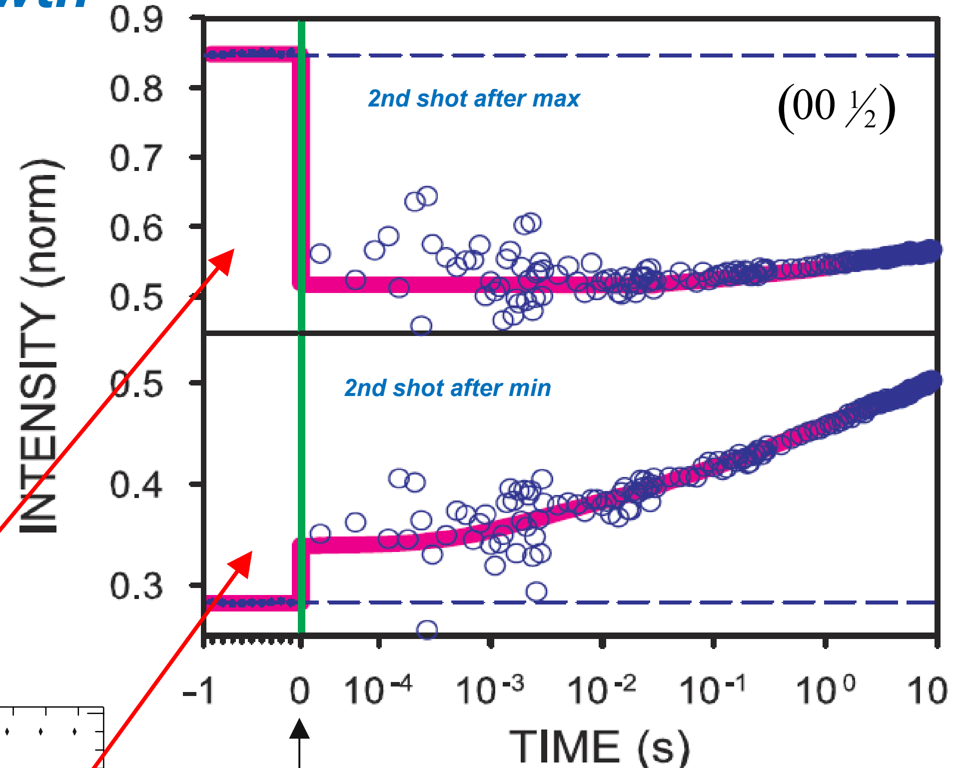
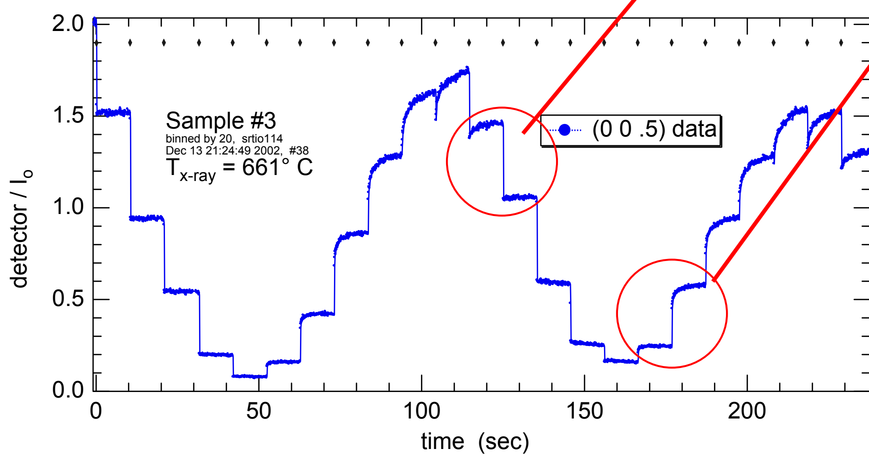
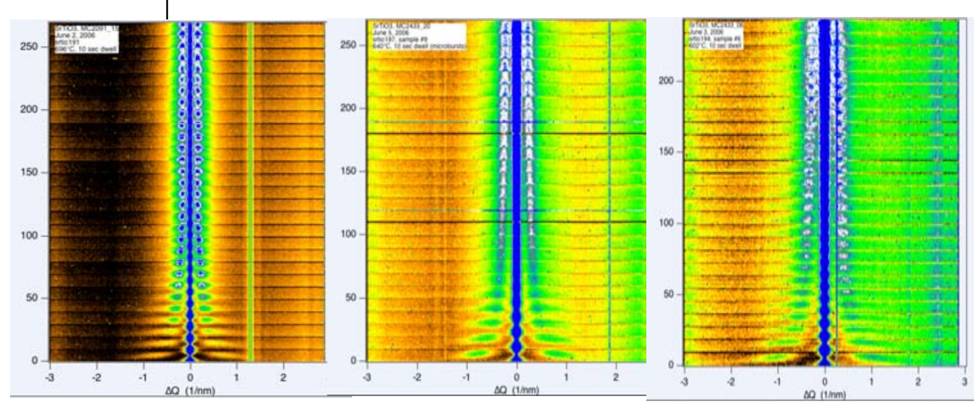


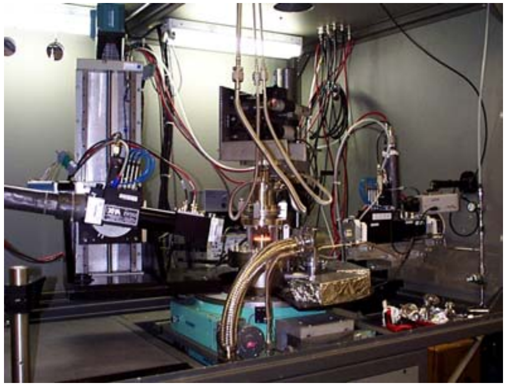


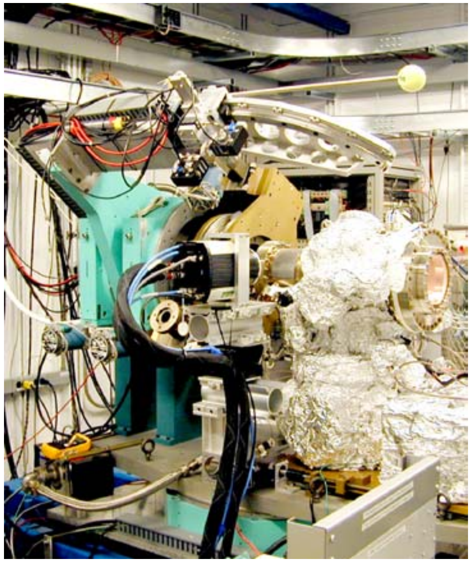


Tischler, et.al. *Phys Rev Lett* **96** (22) 226104 (2006)

Need for In-Situ Facilities

- Many important scientific and technological problems can only be solved by real-time, *in situ* analysis
- Solving these problems requires concentrated, dedicated, complex experiments in a sophisticated facility
- The upgrade of the APS is a great opportunity to create a unique *in situ* facility.



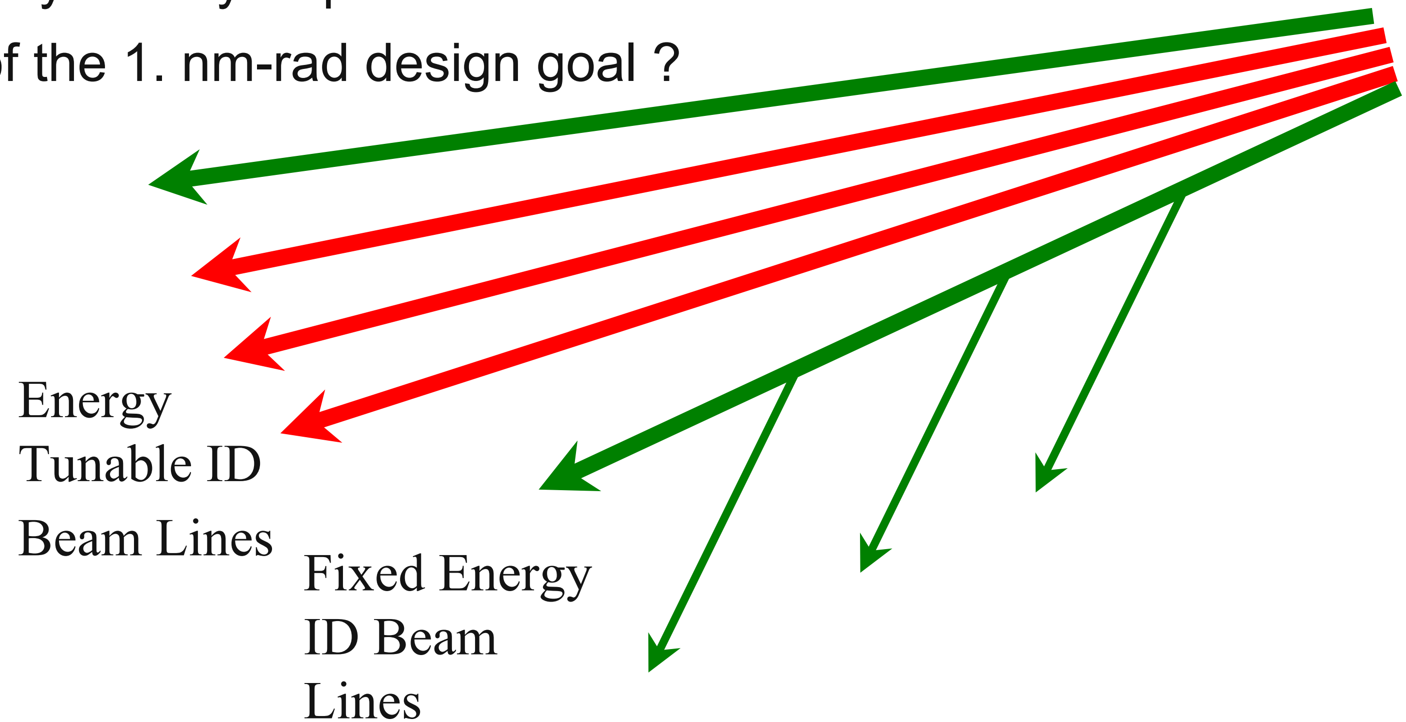


Considerations for In-Situ Capabilities at APS

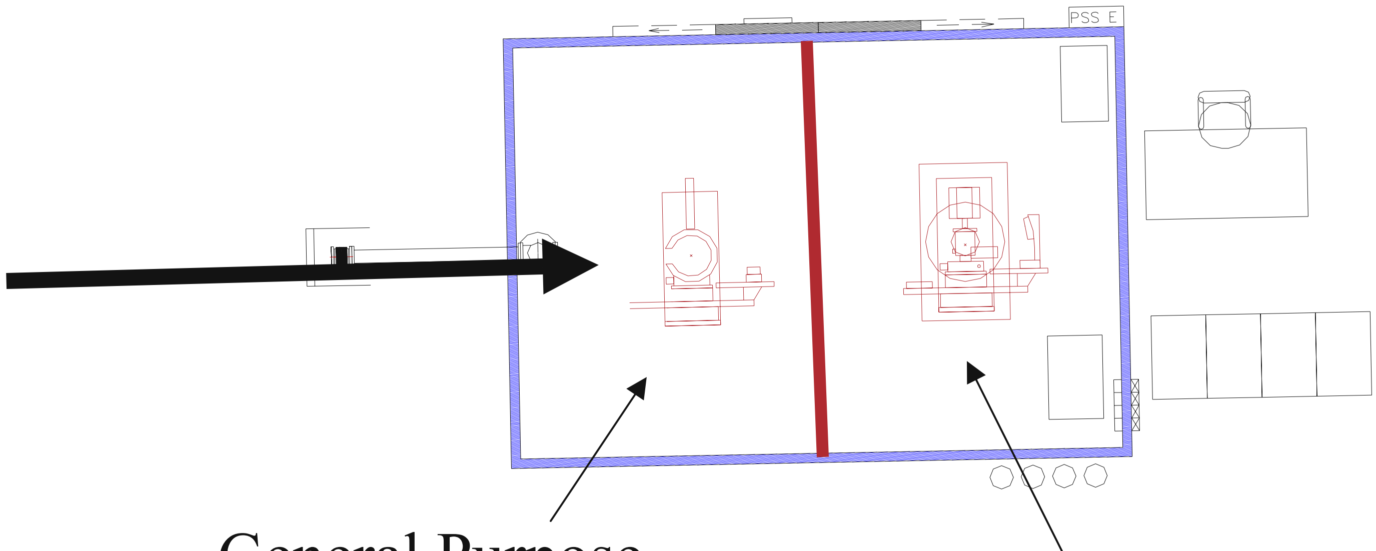
- Synergistic location
  - Co-locate techniques with complementary requirements
  - High overhead experiments at end of line, easy to insert experiments upstream
- Canted undulators
  - Twice as many undulators per sector
  - Synergistic location is difficult
- Multiplexed operation
  - requires restricted operating ranges
- High density sectors
  - Greatly increased number of beamlines
  - Sector feeds dedicated facilities with enhanced capabilities

Concept for a High-Density Insertion Device Sector

- 4 – 5 straight sections for IDs (each 1 – 1.5 m long)
- Bend magnet source converted to ID (APSx3)
- Energy tunable beam lines
- Fixed and/or multiplexed beam lines (with optimized ID)
- Storage ring symmetry required
- Relaxation of the 1. nm-rad design goal ?



Compatible End-Station Capabilities



General Purpose
Diffractometer

Specialized System

New Opportunities in Surface and Interfacial Science

- Surface and Interfacial structure is critical in many disciplines and important materials systems
- XRIM and other imaging techniques will be integrated with other traditional surface & interface scattering techniques to revolutionize our understanding of buried interfaces
- Time-resolved growth investigations will permit understanding of the earliest stages of non-equilibrium PLD growth, leading to improved high-quality film growth
- An In-Situ Materials Creation, Processing, and Characterization facility will enable new dedicated in-situ measurement capabilities to extend knowledge in materials growth and processing and impact diverse scientific areas ranging from energy and communications to environmental and geochemical sciences

Acknowledgements

- *Paul Fenter*
- *Paul Fuoss*
- *Jon Tischler*
- *135 Workshop Participants*
- *35 Planning Meeting Participant*